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EXPERIMENTAL INVESTIGATION OF THE REPRESENTATIVE VOLUME ELEMENT SIZE

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Abstract

In this investigation, the minimum size of the representative volume element (RVE) of a heterogeneous material is determined experimentally using the digital image correlation (DIC) technique. The uniaxial compression experiment was conducted on the PBS 9501, a high explosive simulant material. The minimum size of the representative volume element (RVE) of the PBS 9501 heterogeneous material, where the average crystal diameter of the material is around 100μm, was determined experimentally to be 1.5mm. This result is consistent with those numerical calculations on polycrystalline materials and some other composites.

Keywords: Representative Volume Element, RVE, and Heterogeneous Materials.

Introduction

Almost all the engineering materials are heterogeneous in nature. They are either compounds composed of several different phases or aggregates of crystals with different sizes and orientations. Theoretical estimation of the macroscopic and overall constitutive behavior of the heterogeneous material plays a central role in many engineering applications. Such theoretical estimates are usually obtained by homogenization processes. At the heart of the homogenization process is the so-called representative volume element, or RVE. In order for the constitutive models, based on the homogenization approach, to accurately describe the overall response of the heterogeneous solids, the minimum size of the representative volume element must be known. Hill (1963) gave the first definition for the representative volume element and later he proposed a more descriptive definition for the RVE that involves a very detailed calculation (Hill, 1967). To perform Hill's calculation requires a very detailed description of the microstructure within the element. Drugan and Willis (1996) adopted another definition for the RVE. They regard a RVE as the smallest material volume element of the heterogeneous solid for which the usual spatially constant "overall modulus" macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive response. Drugan and Willis (1996) studied the minimum RVE size of an elastic composite composed of a random dispersion of non-overlapping identical spheres. Gusev (1997) investigated the same problem numerically. For any realistic heterogeneous material with a random microstructure, determining the minimum size of the RVE remains an open question.

In this study, we conducted experimental investigations to study the nature of heterogeneity and to determine the minimum size of the RVE for a heterogeneous material, PBS 9501, a high explosive simulant material. The experiment was uniaxial compression, where an overall uniform deformation is applied to the sample. Using the digital image correlation (DIC) technique, we were able to measure the strain field under a fixed externally applied load. The results of our measurement depend on the material element size used in the digital image correlation calculation. We found that when the material element exceeds a certain size, the mean value of the distribution of strain converged to a constant. Meanwhile, the scatter of strain data becomes smaller when the material element size increases. By examining the variation of the mean value of strain, as a function of the material element size, the minimum size of the RVE for PBS 9501 simulant was determined. Implications of these observations and measurements will be discussed.

Digital Image Correlation (DIC) Technique

Digital image correlation technique relies on the computer vision approach to extract the whole-field displacement data, that is, by comparing the features in a pair of digital images of a specimen surface before and after deformation. Since a feature in the digital image correlation technique (DIC) was explored in our experimental study, a brief description of the underlying principle of the DIC technique is given below.

Consider a planar object illuminated by a light source and suppose that the object undergoes planar deformation. Let R be a small region of the undeformed two-dimensional object and R_* be the same region but in the deformed configuration. The light intensity pattern of the undeformed region R is denoted by $I(\mathbf{x})$ where $\mathbf{x} \in R$, while the light intensity pattern of the deformed region R_* is denoted as $I_*(\mathbf{y})$ where $\mathbf{y} \in R$ and $\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x})$. Both $I(\mathbf{x})$ and $I_*(\mathbf{y})$ are assumed to be in unique and one-on-one correspondence with the respective object surface, and they are integer-valued functions ranging from 0 to 255 when using an 8-bit gray-scale digital camera. If during the deformation process, the intensity pattern only deforms but does not alter its local value, then we should have

$$I_*(\mathbf{y}) = I_*(\mathbf{y}(\mathbf{x})) = I(\mathbf{x}), \quad \forall \mathbf{x} \in R. \tag{1}$$

As a result, the measurement of the displacement field using the digital image correlation technique can be formulated into the following mathematical problem: By knowing the two intensity patterns $I(\mathbf{x})$ and $I_*(\mathbf{y})$ of the same region before and after deformation, find a mapping relation

$$\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x}), \tag{2}$$

such that

$$I_*(\mathbf{y}(\mathbf{x})) - I(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in R. \tag{3}$$

Furthermore, if the deformation is *homogeneous*, or if the deformation is such that

$$\hat{\mathbf{y}}(\mathbf{x}) = \mathbf{F}\mathbf{x} + \mathbf{b}, \tag{4}$$

where $\mathbf{F}$ is a constant tensor and $\mathbf{b}$ is a constant vector, and for two-dimensional deformation, the components of $\mathbf{F}$ and $\mathbf{b}$ in an orthonormal coordinate system can be written as

$$\mathbf{F} = \begin{bmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \tag{5}$$

the above mathematical problem becomes to find a tensor $\mathbf{F}$ with four scalar components, and a vector $\mathbf{b}$ with two components, such that

$$I_*(\mathbf{F}\mathbf{x} + \mathbf{b}) - I(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in R, \tag{6}$$

with the restriction of $\det \mathbf{F} = f_{11}f_{22} - f_{12}f_{21} > 0$. Once the deformation gradient tensor for two-dimensional deformation $\mathbf{F}$ is determined, the strain within the region R can be calculated. For example, the Green-Lagrangian strain tensor E can be calculated by

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{I}), \tag{7}$$

where $\mathbf{I}$ is the identity tensor. Detailed descriptions regarding the DIC technique can be found in Chu *et al.* (1985), Bruck *et al.* (1989) and Vendroux and Knauss (1998).

Note that any general deformation can always be viewed as locally homogeneous provided that the region R considered is sufficiently small. On the other hand, for any given size of the material element R, the strain tensor obtained through the digital image correlation, as given in Eq. (7), represents an average strain that the material element R is experiencing. Now consider a sample made of a heterogeneous material and the sample is subjected to a uniform boundary condition $u_i = \varepsilon_{ij}x_j$, where u_i is the displacement, x_i is position, and ε_{ij} is the strain tensor within the sample if it is made of a homogeneous material. Suppose that we are measuring the strain field within the sample using the digital image correlation technique described above. When the size of the material element R used in the calculation is small, one would expect that the measured average strain of the element R is different from ε_{ij} due to the heterogeneous nature of the material. Only when the size of the material element R becomes sufficiently large, the measured average strain of the element R will approach the applied strain ε_{ij}. By examining the variation of the measured average strain of the element R as a function of the size of the element R, the minimum size of the representative volume element (RVE) of the tested heterogeneous material can be determined. Similar concept was also employed by Ren and Zheng (2002) in their numerical study of the minimum sizes of representative volume elements of cubic polycrystals by monitoring the variation of the nominal modulus tensor as a function of the size of a finite volume.

Experimental Observations and Results

A high explosive simulant material, referred to as PBS 9501, was used in the present investigation. The reason of choosing such a material is that PBS 9501 can simulate, at the macroscopic level, the mechanical behavior of the PBX 9501 high explosive, which is composed by the HMX energetic crystal and a polymeric binder, as a function of strain rate and temperature. Also, the sugar crystal and the HMX crystal are both monoclinic, so they are similar microscopically as well. Both the PBS 9501 and the PBX 9501 have the same polymeric binder system. A micrograph of the PBX 9501 high explosive is shown in Fig. 1. Note that the HMX crystal has a very wide range of spectrum in sizes and the average diameter is about 100μm. The PBS 9501 simulant is composed of 94wt% C&H granulated sugar crystals and 6wt% polymeric binder, which in turn, is composed by 50% estane and 50% nitroplasticizer.

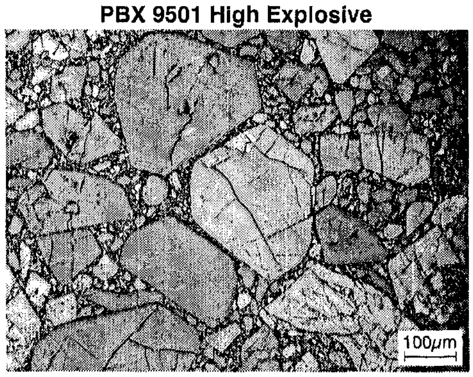
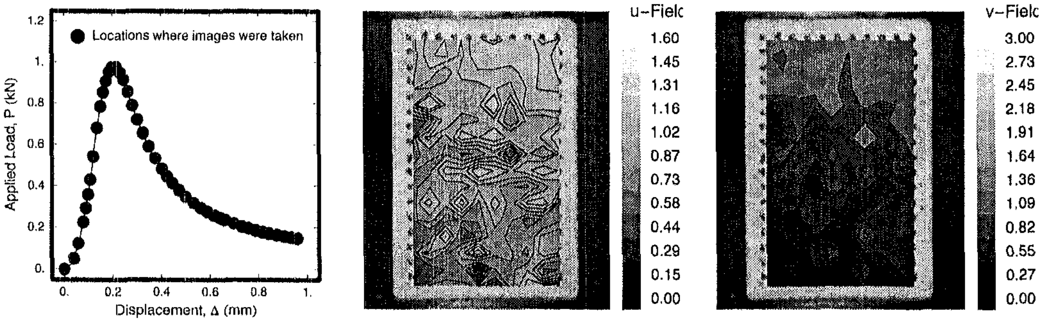


Figure 1. Micrograph of the PBX 9501 high explosive.

The specimen we studied has a rectangular shape with the width of 12.7mm and the thickness of 12.7mm. The height of the specimen is 19.0mm. The specimen was loaded in compression at an equivalent strain rate of 1.7×10^{-4} $\sec^{-1}$. Variation of the applied load as a function of the displacement for the uniaxial compression test is presented in Fig. 2(a), where the solid circles represent the moments when the images of the specimen were taken. These digital images were used later in the digital image correlation calculations to determine the deformation field at different loading stages. Using the digital image correlation technique described in the previous section, the

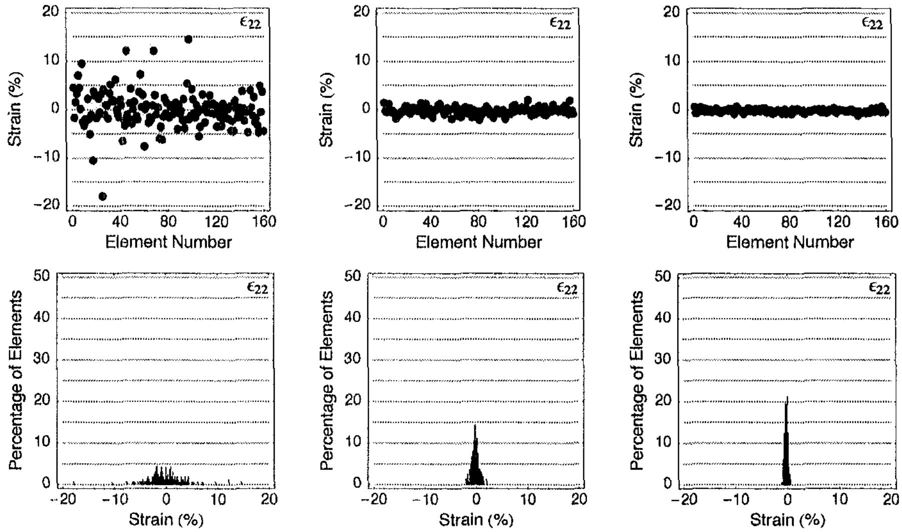


(a) (b)

Figure 2. (a) Variation of applied load versus displacement and (b) displacement field within the sample at P=400N.

deformation field within the compressive sample can be determined. In Fig. 2(b), the contour plots of the two displacement components are shown for the applied load $P = 400\text{N}$.

To determine the minimum size of the representative volume element of the heterogeneous material, we also calculate the strain distribution on the surface of the compressive sample. A matrix of 160 points were chosen on the sample surface and the digital image correlation calculations were carried out on those points. We also chose an image of the deformed sample at the early loading stage so that the deformation is in the elastic range and the strain measurement is not affected by damage or some other deformation mechanisms due to applied load. As we have mentioned in the previous section, the deformation measurement using the DIC technique depends on the size of the small region or the material element R. In Fig. 3, the measurement results of the strain component along the loading direction, ε_{22}, are presented for three different sizes of R used in the correlation calculations. For each



(a) (b) (c)

Figure 3. DIC results of the strain components along loading direction, ε_{22}, for different material element sizes: (a) 0.45mm, (b) 0.90mm, and (c) 1.35mm.

element size, the upper plot in Fig. 3 shows the strain measurement at all the 160 points and the lower plot shows histogram, which also resembles the distribution density of the measured strain of all the 160 elements. For small material element, the measured strain scatters over a wide range. As seen in Fig. 3(a), when the material element size is 0.45mm, the component ε_{22} scatters from –18% to 15%, even though the element size is about 4 to 5 times of the average crystal diameter. As the size of the material element increases, the scatter of the measured strain decreases as shown in Figs. 3(b) and 3(c).

In Fig. 4(a), the mean values of all three in-plane strain components, together with their standard deviations, are presented as a function of different material element sizes ranging from 0.45mm to 2.25mm. One can see that the standard deviation is quite large for small material element and decreases rapidly as the material element size increases. For material elements larger than 1.5mm, the standard deviation almost no longer changes. This stabilized standard deviation actually characterizes the uncertainties of the experimental technique itself and no longer represents the heterogeneous nature of the material. As a result, we may assign the length above which the heterogeneity does not affect the deformation measurement any more, as the minimum size of the representative volume element. An alternative way for determining the minimum RVE size is to look at the convergence of the mean value of the measured strain components. In Fig. 4(b), only the mean value of all three in-plane strain components is plotted against the size of the material elements. Once again, as we discussed in the previous section, for smaller material elements, the

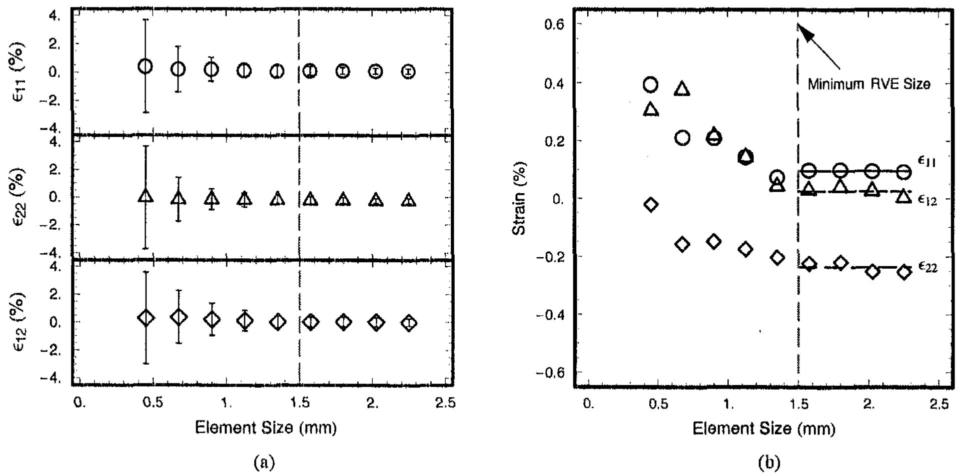


Figure 4. (a) Variation of the mean value and the standard deviation (as error bars) of measured strain as a function of material element size. (b) Convergence of the strain component when material element size increases.

mean value of the measured strain changes rapidly and this is the case for all three in-plane strain components obtained using the digital image correlation technique. However, for material elements larger than 1.5mm, each of the all three in-plane strain components converges to a constant. Moreover, the strain component along the loading direction, ε_{22}, actually converges to the value of the strain imposed from the boundary condition of the compressive sample. Therefore, we can conclude that the minimum size of the representative volume element for the heterogeneous PBS 9501, is about 1.5mm.

Concluding Remarks

In this study, we investigated experimentally the minimum size of the representative volume element of the heterogeneous material PBS 9501, a simulant of the PBX 9501 high explosive. Using the digital image correlation technique, we were able to determine that the minimum RVE size of the PBS 9501 is approximately 1.5mm. This length is about 15 times of the average diameter of the crystals of the material. In a two-dimensional region, an RVE would include at least 250 crystals assuming that all the crystals have the same size as the average diameter, so that the response of the element can represent the overall mechanical behavior of the PBS 9501. This result is consistent with the observation of other numerical studies. For example, Elvin (1996) studied the number of grains required to represent the homogeneous elastic behavior of polycrystalline ice. He considered fresh water, columnar-grained ice with relatively uniform grain size. Elvin found that, in two dimensions, at least 230 grains are needed to homogenize the elastic properties. He also found that the sliding condition along grain boundaries would influence the RVE size. In another numerical study, Ren and Zheng (2002) obtained the minimum RVE sizes for more than 500 kinds of cubic polycrystalline materials. Once again, they assumed that all the crystals have the same size, so that only the effect of crystal orientations was considered. They concluded that the minimum RVE size is about 20 times of the crystal size, which translates into that for a two-dimensional RVE, there are about 400 crystals in it. As can be seen in Fig. 1, the material we considered in this investigation is a lot more complicated than those considered in numerical studies. Meanwhile, even though we only measured the in-plane strain field, the deformation in the third direction definitely also affects the determination of the minimum RVE size in our experimental study.

We also need to point out that the minimum RVE size not only is material dependent, but also is material-property dependent. As proved by Nye (1957), that the linear thermal conductivity of any cubic crystal is always isotropic, but the linear elasticity is anisotropic. As a result, for cubic polycrystal, the minimum RVE size for linear conductivity might be different from that for linear elasticity. Since we based our minimum RVE size determination on measuring deformation of the material under externally applied mechanical load, the minimum RVE size we obtained in this study is associated with the mechanical response of the material. Moreover, since we concentrated on the early stage of loading, where deformation is small, the minimum RVE size is ultimately related to the elastic behavior of the material.

Acknowledgements

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